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Infrared spectra of C6–spiro steroidal tetrazines

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Abstract Chloro, Bromo, Iodo and Acetate derivatives of C6 - spiro steroidal tetrazine, have been prepared Infrared spectra of these derivatives and the parent compound have been recorded in the range 650–4000 cm^{-1} Vibrational analysis has been performed in terms of various fundamental vibrations and combinations of these vibrations These compounds exhibit some interaction vibrations, which indicate the nature of complexities in such big molecules Assignments of all the observed frequencies are proposed and thermodynamic functions calculated for a few temperatures in the range from 100 to 1500 K

Keywords Infrared spectra, thermodynamic functions, steroidal spiro tetrazines, vibrational analysis

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1. Introduction

Steroids were first developed in 1930's. The Germans first experimented on dogs then on their own soldiers in the Second World War, as well as then on their prisoners to help them stay healthy [1]. Then in 1950's many Russian and European athletes began to find that steroids were very beneficial to their goal. A decade later steroids were used in medicine, as steroids are medicinal compound exhibiting a lot of potentialities to form other complicated organic compounds, which are more useful in the complex diseases. Infrared spectra of steroids are complex due to the fact that its structure is not a simple and uniform one. We have to analyse the infrared spectra by indirect methods namely, selecting the known fundamentals and combination of these fundamentals. Most of the time, these fundamentals and combinations explain the occurrence of interaction vibrations, hydrogen-bonding vibrations and other conformation vibrations. These complicated vibrations should be very carefully identified on the basis of their intensities, their occurrence with various fundamentals and their approximate magnitudes.

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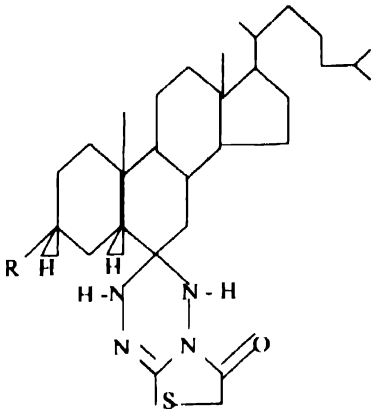
2. Experimental technique

The above compounds have been prepared in Steroidal Research Laboratory, Department of Chemistry, A.M.U. Aligarh [2], and these compounds were used as such with KBr in the form of a circular disc to record the infrared spectra. Infrared spectra were recorded on Perkin-Elmer model – 237 infrared spectrophotometer. The appearance of the spectra is quite good and sharp. Five infrared spectra are being reported here. They have been reproduced in the separate sheet of paper. Vibrational frequencies have been reported with the accuracy of ± 5 cm^{-1}. All infrared spectra have been recorded in the region 600-4000 cm^{-1}. Visual estimates of the intensities have been given in the visual scale of 1 to 10. About 35 to 60 bands have been obtained in each infrared spectrum.

3. Structural formula



R = (H, Cl, Br, I, and OAc)

(i) 6' (7' H)-oxo spiro [5α – cholestan] 6, 3' (4'H)-[2H) Thiazolo [3, 2-b]–5–tetrazine. (or) [C6-SPT]

(ii) 6' (7' H)-oxo spiro [3β- Chloro-5α – cholestan] 6, 3' (4' H)-[2H] Thiazolo [3, 2-b] – 5 – tetrazine. (or) [C6 – Chloro SPT]

(iii) 6' (7' H)-oxo spiro [3β- Bromo-5α - cholestan] 6, 3' (4'H)-[2H] Thiazolo [3, 2-b]–5–tetrazine. (or) [C6 – Bromo SPT]

(iv) 6'(7' H)-oxo spiro [3β-Iodo-5α - cholestan] 6, 3' (4'H)-[2H] Thiazolo [3, 2-b] – 5 –tetrazine. (or) [C6–Iodo SPT]

(v) 6'(7' H)-oxo spiro [3β- acetoxy-5α - cholestan] 6, 3' (4'H)-[2H] Thiazolo [3, 2-b]–5–tetrazine. (or) [C6–Acetoxy SPT]

4. Discussion and analysis

Chloro, bromo, iodo, and acetate derivatives of C6–spiro–steroidal tetrazines have been reproduced in the form of their molecular structure containing various benzene rings. These rings are in association with various molecular bonds. H in the position of 3β has been replaced by Chlorine, Bromine, Iodine and acetate group. All the four derivatives and the parent molecule belong to C_s point group because there is only one plane of symmetry *i.e.* plane of molecule. There will be only two types of vibrations that are a' (planer) and a" (non-planer). The observed fundamental frequencies and probable assignments are presented in Tables 1 to 5.

A.R.H. Cole and his Collaborators [3-5] suggested angular methyl group bending vibrations for the methyl group in between two six-membered rings (C_{10}) and in between a five and a six-membered rings (C_{18}) within the region (1374-1392) cm^{-1} and (1372-1383) cm^{-1} respectively. The bands observed at 1385, 1370 cm^{-1} in (C6-SPT), 1380, 1375, cm^{-1} in (Chloro C6-SPT), 1390, 1365, cm^{-1} in (Bromo C6-SPT), 1390, 1375, cm^{-1} in (Iodo C6-SPT), and 1385, 1375, cm^{-1} in (Acetoxy C6-SPT), have been assigned for angular methyl bending vibrations in methyl group in between two-six membered rings and in between five and six membered rings respectively.

In the steroidal series, a limited number of compounds have been studied, and the results indicate that equatorial substitution leads to bands in the (750–700 cm^{-1}) region, whereas axial substitution results in absorption in the (590–690 cm^{-1}) range [6]. The bands observed at 650 cm^{-1} and 720 cm^{-1} have been

Table 1. Observed infrared frequencies for 6'(7' H)–oxo spiro [5α-cholestan] 6,3' (4'H)–[2H thiazolo [3, 2-b]–5–tetrazine.

I R frequency (in cm^{-1})	Int.	Species	Assignment
685	5 8	a'	C – S stretching
705	6.5	a"	C – H bending o.o.p
730	6.7	a"	C – H bending o.o.p
750	5.9	a"	C – H bending o.o.p
1065	6 7	a"	C – CH_3 rocking
1120	3.4	a'	C – H bending i.p.
1140	5.8	a'	C – H bending i.p.
1205	6.4	a'	C – H bending i.p.
1240	6.1	a'	C – H bending i.p.
1260	6.3	a'	C – N stretching
1305	4 2	a'	C – H bending i.p
1370	4.2	a"	angular methyl group between a five and a six membered ring C_{18}
1385	3.6	a"	angular methyl group between two six membered rings C_{10}
1435	3 3	A', A"	(705 + 730), (685 + 750)
1470	2 7	a"	CH_3 out of phase deformation
1630	3 2	a'	C = N linkage
1760	6 6	a'	C = O stretching
1795	6 8	A'	(730 + 1065)
2070	6 9	A"	(685 + 1385)
2100	6 8	A'	(730 + 1370)
2130	6 7	A'	(2 × 1065)
2240	6 5	A'	(1120 + 1140)
2500	6 4	A'	(1240 + 1260)
2880	1 3	a'	CH_3 in phase stretching
2940	0 7	A'	(2 × 1470)
2955	0.8	a"	CH_3 out of phase stretching
3080	3 8	a'	C – H stretching
3100	3 7	A"	(1470 + 1630)
3140	3 2	a'	C –H stretching
3260	3 9	A'	(2 × 1630)
3440	5 5	a'	N – H stretching
3570	6.8	A'	(2880 + 685)
3630	6.1	A"	(750 + 2880)
3640	6.1	A"	(685 + 2955)
3890	6.0	A"	(750 + 3140)

Table 2. Observed infrared frequencies for 6'(7' H)–oxo spiro [5α–cholestan] 6,3' (4'H)–[2H thiazolo [3, 2-b]–5–tetrazine.

I.R. frequency (in cm^{-1})	Int	Species	Assignment
620	6.4	a'	C – Cl axial stretching
700	5.6	a'	C – S stretching
720	6.4	a"	C – H bending o.o.p
730	6.4	a"	C – H bending o.o.p
750	5.8	a"	C – Cl equatorial stretching
765	5.6	a"	C – H bending o.o.p
1060	6.5	a"	C – CH_3 rocking
1080	5.3	a'	C – H bending i.p.
1110	5.3	a'	C – H bending i p
1150	5.8	a'	C – H bending i p.
1210	6 5	a'	C – H bending i p
1240	6 3	a'	C – H bending i.p.
1260	6 2	a'	C – N stretching
1310	6 2	a'	C – H bending i.p
1340	5 4	A"	(620 + 720)
1375	5 0	a"	angular methyl group between a five and a six membered ring C_{18}
1380	5 7	a"	side chain methyl group
1390	4 6	a"	angular methyl group between two six membered rings C_{10}
1450	3 7	A', A"	(705 + 730), (700 + 750)
1470	3.1	a"	CH_3 out of phase deformation
1500	6 0	A'	(2 × 750)
1610	1 0	a'	C = N linkage
1680	2 0	A'	(620 + 1060)
1740	4 3	a'	C = O stretching
1760	5 1	A'	(700 + 1060)
1810	5 3	A', A", A"	(700 + 1110), (730 + 1080), (1060 + 750)
1825	5 3	A'	(765 + 1060)
1880	5 4	A", A'	(730 + 1150), (620 + 1260)
1960	5 4	A', A', A"	(700 + 1260), (720 + 1240), (1210 + 750)
1990	5 3	A", A"	(700 + 1260), (1240 + 750)
2040	5 2	A"	(700 + 1310)
2110	5 3	A', A'	(720 + 1390), (730 + 1380)
2200	5.2	A'	(730 + 17470)
2420	5 1	A', A'	(2 × 1210), (1110 + 1310)
2610	5 0	A"	(1260 + 1380)
2720	4.7	A'	(1110 + 1610)
2850	2.6	A'	(1380 + 1470)
2870	2.2	a'	CH_3 in phase stretching
2920	2.0	A'	(1310 + 1610)
2960	1.5	a"	CH_3 out of phase stretching
3045	4 1	a'	C – H stretching
3100	3 6	a'	C – H stretching
3420	4.2	a'	N – H stretching
3620	4.8	A"	(750 + 2870)
3660	4.8	A"	(700 + 2960)

Table 3. Observed infrared frequencies for 6'(7' H)–oxo spiro [3β-bromo-5α–cholestan] 6,3' (4'H)–[2H] thiazolo [3, 2-b]–5–tetrazine.

I.R. frequency (in cm^{-1})	Int.	Species	Assignment
650	7.5	a'	C – Br stretching axial
700	7.5	a'	C – S stretching
705	7 4	a"	C – H bending o o.p
720	7.3	a"	C – Br stretching equatorial
750	7.3	a"	C – H bending o.o.p
770	7 1	a"	C – H bending o.o.p
1060	6 4	a"	C – CH_3 rocking
1075	6.1	a'	C – H bending i.p
1115	2 8	a'	C – H bending i.p
1145	5.9	a'	C – H bending i p
1210	4 4	a'	C – H bending i.p.
1225	2 9	a'	C – H bending i p
1265	4 4	a'	C – N stretching
1315	5 8	a'	C – H bending i p
1365	3 6	a"	angular methyl group between a five and a six membered ring C_{18}
1390	1.5	a"	angular methyl group between two six membered rings C_{10}
1480	5 3	a"	CH_3 out of phase deformation
1615	0.3	a'	C = N linkage
1730	1.1	a'	C = O stretching
1845	8 5	A', A"	(700 + 1145), (770 + 1075)
1930	8 2	A", A"	(705 + 1225), (720 + 1210)
1970	7.9	A"	(705 + 1265)
1995	7.8	A"	(770 + 1225)
2020	7.6	A"	(705 + 1315)
2040	7 5	A"	(650 + 1390)
2140	7 0	A'	(750 + 1390)
2160	7 1	A'	(770 + 1390)
2180	7 0	A"	(700 + 1480)
2300	6 5	A'	(1075 + 1225)
2460	6 2	A'	(1145 + 1315)
2540	5 8	A', A'	(1060 + 1480), (1225 + 1315)
2680	5.5	A"	(1315 + 1365)
2860	4.6	a'	CH_3 in phase stretching
2940	3.8	a"	CH_2 asy. stretching
2970	4.4	a'	CH_3 out of phase stretching
2980	4 3	A"	(1365 + 1615)
3040	4 5	a'	C – H stretching
3090	4 3	a'	C – H stretching
3120	3 9	a'	C – H stretching
3150	3.5	a'	C – H stretching
3210	2.8	A"	(1480 + 1730)
3430	4.3	a'	N – H stretching
3460	4.3	A"	(2 × 1730)
3500	4.2	A"	(1730 + 770)
3620	4 8	A"	(650 + 2970)
3660	5.1	A'	(720 + 2940)
3720	5.1	A'	(750 + 2970)
3790	4.9	A', A"	(700 + 3090), (750 + 3040)
3920	4.8	A", A"	(770 + 3150), (1060 + 1860)

Table 4. Observed infrared frequencies for 6'(7' H)-oxo spiro [3β-iodo-

I R frequency (in cm^{-1})	Int	Species	Assignment
670	6 5	a'	C – I stretching
700	6.3	a'	C – S stretching
710	6 6	a"	C – H bending o o p
735	6 5	a"	C – H bending o o p
780	6 0	a"	C – H bending o o p
1065	4 2	a"	C – CH_3 rocking
1080	4 1	a'	C – H bending i p
1105	4 1	a'	C – H bending i p
1140	4 3	a'	C – H bending i p
1195	4 7	a'	C – H bending i p
1240	4 6	a'	C – H bending i p
1260	4 7	a'	C – N stretching
1305	5 6	a'	C – H bending i p
1375	5 8	a"	angular methyl group between a five and a six membered ring C_{18}
1390	4 4	a"	angular methyl group between two six membered rings C_{10}
1405	5 0	A"	(670 + 735)
1470	5 2	a"	CH_3 out of phase deformation
1515	6 1	A'	(735 + 780)
1560	5 8	A'	(2 × 780)
1640	3 4	a'	C = O Linkage
1735	4 1	A"	(670 + 1065)
1750	4 8	A'	(670 + 1080)
1775	6 1	A', A'	(670 + 1105), (710 + 1065)
1780	6 3	a'	C = O stretching
1865	6 4	A'	(670 + 1195)
1895	6 3	A'	(700 + 1195)
2040	6 1	A"	(735 + 1305)
2080	6 2	A", A'	(780 + 1260), (710 + 1375)
2140	6 2	A"	(670 + 1470)
2170	6 0	A"	(700 + 1470)
2185	6 1	A'	(1080 + 1105)
2220	6 0	A'	(1080 + 1140)
2250	6 0	A'	(780 + 1470)
2310	5 8	A'	(670 + 1640)
2350	5 9	A"	(710 + 1640)
2380	5 8	A'	(1140 + 1240)
2480	5 8	A'	(2 × 1240)
2490	5 8	A"	(1105 + 1390)
2720	5 4	A'	(1080 + 1640)
2780	5 4	A'	(1140 + 1640)
2875	2 8	a'	CH_3 in phase stretching
2920	2.4	A'	(1140 + 1780)
2945	1 8	a"	CH_2 asy, stretching
2960	1 4	a"	CH_3 out of phase stretching
3015	4 3	a'	C – H stretching
3025	4 7	a'	C – H stretching
3125	5 0	a'	C – H stretching
3170	5.1	A"	(1390 + 1780)
3250	4.8	A'	(1470 + 1780)
3420	4 7	a'	N – H stretching
3440	4 6	a'	N – H stretching
3610	5 2	A"	(735 + 2875)
3740	5 5	A'	(780 + 2960)
3790	5 7	A"	(780 +3015)
3840	5 4	A"	(710 + 3125)

Table 5. Observed infrared frequencies for 6'(7' H)–oxo spiro [3β-acetoxy-5α-cholestan] 6,3' (4'H)–[2H] thiazolo [3, 2-b]–5–tetrazine.

I.R frequency (in cm^{-1})	Int	Species	Assignment
695	4.5	a'	C – S stretching
710	2.6	a"	C – H bending o.o.p
730	4.5	a"	C – H bending o.o.p
770	2 8	a"	C – H bending o.o.p
1065	3.2	a"	C – CH_3 rocking
1085	2 1	a'	C – H bending i.p
1110	2 0	a'	C – H bending i.p
1145	3.8	a'	C – H bending i.p
1180	3 1	a'	C – H bending i.p
1220	3 7	a'	C – H bending i p
1260	0 0	a'	C – N stretching
1310	3 3	a'	C – H bending i p
1340	3.2	a'	C = O stretching
1375	1 1	a"	angular methyl group between a five and a six membered ring C_{18}
1385	0 7	a"	angular methyl group between two six membered rings C_{10}
1470	0.8	a"	CH_3 out of phase deformation
1610	1.1	a'	C = N linkage
1730	0 2	a'	carbonyl stretching in between acetoxy group and a six membered ring
1775	3 1	a'	C = O stretching
1910	5.7	A"	(730 + 1180)
1950	5.8	A"	(770 + 1180)
2020	5 8	A"	(710 + 1310)
2180	5.7	A'	(710 + 1470)
2290	5 8	A'	(1110 + 1180)
2440	5.7	A', A'	(710 + 1730), (2 × 1220)
2460	5:6	A', A"	(730 + 1730), (1085 + 1375)
2500	5 6	A'	(770 + 1730)
2520	5.5	A",A',A'	(1145 + 1375), (1340 + 1180) (1220 + 1260)
2560	5.5	A'	(1220 + 1340)
2780	4 9	A"	(1310 + 1470)
2870	0 5	a'	CH_3 in phase stretching
2940	0.2	a"	CH_2 asy, stretching
2960	0.0	a"	CH_3 out of phase stretching
3040	2.5	a'	C – H stretching
3080	2.2	a'	C – H stretching
3110	2.1	a'	C – H stretching
3140	2.0	a'	C – H stretching
3200	1.9	A'	(1470 + 1730)
3430	3.1	a'	N – H stretching
3600	4.3	A"	(730 + 2870)
3640	4.6	A"	(700 + 2870)

Table 6. Calculated values of thermodynamic functions (in cal/mol/°K)

	C6-SPT Zero point energy = 54.336 × 10^3 cal/mol/°K				Chloro C6-SPT Zero point energy = 54 371 × 10^3 cal/mol/°K				Bromo C6-SPT Zero point energy = 65 576 × 10^3 cal/mol/°K				Iodo C6-SPT Zero point energy = 64.947 × 10^3 cal/mol/°K				Acetoxy C6-SPT Zero point energy = 64 947 × 10^3 cal/mol/°K			
Temp °K	X = hωc/kT	Enth	Heat Cap	(−)Free energy	X = hωc/kT	Enth	Heat Cap	(−)Free energy	X = hωc/kT	Enth	Heat Cap	(−)Free energy	X = hωc/kT	Enth	Heat Cap	(−)Free energy	X = hωc/kT	Enth	Heat Cap	(−)Free energy
100	547.108	0.0029	0 0292	0.00027	547.468	0.0053	0.0514	0 00054	660 285	0 0047	0.0472	0.00046	653 954	0 0037	0.0374	0.00037	684.029	0.0026	0 0267	0.00025
200	273.554	0.274	1.540	0.051	237 734	0 412	2.205	0 079	330 143	0.402	2.171	0 076	326 977	0.335	1.836	0.063	342.014	0.264	1.498	0.048
300	182.369	1.337	5.735	0.334	182 489	1.801	7 251	0 478	220 095	1.771	7 120	0.468	217 985	1 529	6.282	0 369	228.010	1.303	5.605	0.324
400	136.777	3.101	11.098	0 948	136 867	3.892	13.059	1.271	165 071	3 811	12.718	1.246	163.488	3.370	11.504	1.077	171.007	3.028	10.852	0.923
500	109.422	5.222	16.216	1 864	109 494	6.268	18 351	2 392	132 057	6 114	17 805	2.342	130 791	5.491	16.342	2 054	136 806	5 110	15.944	1.818
600	91 185	7.431	20.560	3.011	91.254	8.663	22 791	3.748	110 048	8.434	22 142	3.662	108 992	7 656	20 513	3 247	114 005	7 299	20.443	2.943
700	78.158	9.581	24.740	4.319	78.210	10.951	26 648	5 257	94 327	10.662	26 162	5.131	93.422	9 754	24.509	4 586	97.718	9.462	24.874	4.231
800	70.955	11.036	26 404	5.316	71.002	12.484	28.612	6.389	85 633	12.167	28 076	6 235	84 812	11 180	26 269	5 598	88.712	10.947	26.723	5.217
900	60.790	13.494	30 043	7.210	60.830	15 049	31.963	8 516	73.365	14 719	31.820	8 311	72 662	13 608	30.016	7 512	76.003	13.498	30.891	7.105
1000	54.711	15.235	31.847	8 723	54 747	16.852	34.036	10 196	66 029	16 542	34.023	9 957	65 395	15.351	32 098	9.037	68.403	15.339	33.051	8.623
1100	49.737	16.839	33.507	10.252	49.770	18.506	35 454	11 881	60 026	18 236	35.824	11 614	59 450	16 976	33.929	10 577	62.184	17 061	35.139	10.167
1200	45.592	18.315	35 223	11.781	45.622	20.022	37 382	13 557	55 024	19 809	37.928	13.269	54 496	18 490	35.941	12 120	57.002	18.667	37.193	11.721
1300	42.085	19.673	36 192	13 301	42.113	21 414	38.131	15 216	50 791	21 270	39 041	14.913	50 304	19 900	37.103	13 656	52.618	20.164	38.541	13.275
1400	39.079	20.926	37.694	14.806	39.105	22 695	39.828	16.850	47 163	22 629	40.896	16.540	46 711	21.213	38 882	15 180	48 859	21.559	40.326	14.821
1500	36 474	22.082	38.753	16.290	36 498	23.874	40.864	18 457	44 019	23.892	42 172	18.145	43.597	22.437	40 154	16.686	45.602	22.585	41.674	16.353

assigned to axial C – Br stretching and equatorial C-Br stretching vibrations in (Bromo C6-SPT) respectively.

Axial C-Cl stretching vibrations and equatorial C-Cl stretching have been observed at 620 cm^{-1} and 750 cm^{-1} respectively in (Chloro C6 -SPT). Barton *et al* [7] has suggested these vibrations near 617 cm^{-1} and 750 cm^{-1} respectively.

Barton, Page, and Shoppee [7], suggested C-I stretching vibrations at 672 cm^{-1} for Iodo- steroidal. The band observed at 670 cm^{-1} in (Iodo C6–SPT), has been assigned to C-I stretching vibration.

The C-S stretching vibration normally appears in the infrared as a weak absorption in the range [8], (700–600 cm^{-1}). The bands observed at 685 cm^{-1} in (C6–SPT), 700 cm^{-1} in (Chloro C6–SPT), 700 cm^{-1}, in (Bromo C6–SPT), 700 cm^{-1} in (Iodo C6–SPT), and 695 cm^{-1} in (Acetoxy C6–SPT) have been assigned to C-S stretching vibrations.

Bellamy [8] and Rao [9] have suggested that N-H stretching vibrations occur in the region (3450–3400 cm^{-1}). In accordance with their conclusions, the bands observed at 3440 cm^{-1} in (C6–SPT), 3420 cm^{-1} in (Chloro C6–SPT), 3440 cm^{-1} in (Bromo C6–SPT), 3420, 3440 cm^{-1} in (Iodo C6–SPT), and 3430 cm^{-1} in (Acetoxy C6 – SPT) have been assigned to N–H stretching vibrations

Several workers [10-12] reported C = O stretching vibrations in five-membered rings for steroids at (1780–1778 cm^{-1}). The observed band at 1760 cm^{-1} in (C6–SPT), 1730 cm^{-1} in (Chloro C6-SPT), 1730 cm^{-1} in (Bromo C6–SPT), 1780 cm^{-1} in (Iodo C6–SPT), and 1775 cm^{-1} in (Acetoxy C6–SPT) have been assigned as C = O stretching vibrations in five membered ring

Hadzi and Skrbljah [13] and Lieber *et al* [14] have suggested C-N stretching vibrations around 1260 cm^{-1} We observed C-N stretching vibrations at 1260 cm^{-1} in (C6–SPT), 1260 cm^{-1} in (Chloro C6–SPT), 1265 cm^{-1} in (Bromo C6–SPT), 1260 cm^{-1} in (Iodo C6–SPT), and 1260 cm^{-1} in (Acetoxy C6–SPT) have correlation with the given assignment.

Lieber *et al* [14] reported a number of C = N conjugated ring compounds and observed a strong absorption at 1626 cm^{-1}, which they assigned to the C = N linkage vibration. The bands observed at 1630 cm^{-1} in (C6–SPT), 1610 cm^{-1} in (Chloro C6–SPT), 1615 cm^{-1} in (Bromo C6–SPT), 1640 cm^{-1} in (Iodo C6–SPT), and 1610 cm^{-1} in (Acetoxy C6–SPT) have been assigned to C = N linkage frequencies.

5. Thermodynamic functions

The thermodynamic functions of pyridine, benzene derivatives, *p* - Fluorobenzyl Alcohol, 2, 3 – dimetoxy toluene, Trifluoromethylbenzoyl Chlorides, 6 – azauracil, 5 – Iodo urcil, 6 – methyl uracil, bio – molecules, have been the subject of many investigators [15-22], as the thermodynamical properties of a molecule may be computed more accurately than measured, using fundamental frequencies of a molecule. Therefore, it was considered worthwhile to study the thermodynamic properties of series of C 6-spiro steroidal tertrazines. The ideal gas state thermodynamic functions are computed in the temperature range 100–1500 K utilizing the spectroscopic data given in Tables (1-5). The numerical values for the thermodynamic functions in ideal gas state as given in Table 6 are computed as described earlier [23-25].

6. Conclusion

Vibrational assignments of such complicated molecules have been performed by taking the help of similar vibrations observed in similar molecules. These studies will be helpful to identify ground state vibrations of the above steroids. In the electronic spectra of the steroids, excited state vibrations can be confirmed with the help of ground state vibrations observed in the infrared spectra of the same molecules.

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